Statistical analysis methods for Particle Physics: Status and Prospects

(from an LHC perspective)

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Randomness in High-Energy Physics



Experimental data is produced by incredibly complex processes!

Randomness in High-Energy Physics

Experimental data is produced by incredibly complex processes



 \rightarrow Quantum effects in production, decay

Quantum Randomness: H→ZZ*→4I



Quantum Randomness: H→ZZ*→4I



Quantum randomness: "Will I get an event today ?" \rightarrow only probabilistic answer

Discoveries



Data

Discoveries ... or not

Randomness \Rightarrow fluctuations.

How to distinguish this from New Physics ?

 \rightarrow ... and robust methods to control **spurious "discoveries"**...



Parameter Measurements

Randomness \Rightarrow Measurement uncertainties

Key point for precision measurements,

⇒ Answers to important questions (especially if no new peaks found at high mass...)



Consistency of the SM...

... or the fate of the universe

Statistical Methods

- Many ways to perform statistical analyses:
 → types of results
 → modeling assumptions
 - \rightarrow available CPU power
- Large experimental efforts ⇒ new developments: LEP, TeVatron, BaBar/Belle, LHC, etc.

• Long term trend:

→ more complex experiments
 → more focus on systematics
 ⇒ more detailed statistical modeling

100 (GeV) mp+0-Events / (20 MeV/c² BABAR 454 fb-1 J^{PC} = 1⁻⁻ 0808.1543 (2008 4.2 4.4 4.6 $m(\pi^+\pi^-J/\psi)(GeV/c^{2})$ CL_s LEP210 √s ≤210 GeV Observed ----- Expected background 115.0

102 104 106 108 110 112 114 116 118

- This talk: (biased) summary of current practices at LHC : → Focus on frequentist interpretation, profiling of systematics
 - → Many aspects relevant also for other methods e.g. Statistical modeling

 $m_H(GeV/c^2)$

Statistical Modeling

Statistical Model

Goal:

Describe the random process by which the data was obtained.

→ Build a Statistical Model



Ingredients:

- Statistical description of the random aspects
 ⇒ Probability distributions
- Assumptions on the underlying statistical processes (physics, etc.)
 → Uncertainties on the assumptions themselves: systematic uncertainties

"Systematic uncertainty is, in any statistical inference procedure, the uncertainty due to the incomplete knowledge of the probability distribution of the observables.

G. Punzi, What is systematics ?

Statistical results can only be as accurate as the model itself !

Modeling Rare Processes: Poisson Counting

Counting experiment:



$$P(n;\lambda) = e^{-\lambda} \frac{\lambda^n}{n!}$$



Typically both signal and background expected:

$$P(n; S, B) = e^{-(S+B)} \frac{(S+B)^n}{n!}$$

S : # of events from signal processB : # of events from bkg. process(es)

 \rightarrow Example: **assume B is known**, use the **measured n** to find out about the **parameter S**. usually up to uncertainties \rightarrow systematics

12



N=1: Back to the simple counting analysis

 \rightarrow Can obtain fractions directly from MC

 \rightarrow MC stat fluctuations can create artefacts, especially for S \ll B.

Model 3: Unbinned Shape Analysis

Observable: event-by-event m,... m,

→ Describe shape of the **distribution of m**

 \rightarrow Deduce the **probability to observe m**₁... m_n



Vormalized events per GeV

0.25

0.2

0.15

0.1

0.05

m

Signal

σ

Н→үү

JHEP 11 (2018) 185



Categories

Multiple analysis regions often used

- \rightarrow Useful to model separately if
- Useful to model separation ... Regions with better sensitivity (avoids dilution)
- Multiple signal measurements

\Rightarrow Analysis categories :

$$P(S; \{n_i^{(k)}\}_{i=1...n_{\text{evts}}}^{k=1...n_{\text{cats}}}) = \prod_{k=1}^{n_{\text{cats}}} P_k(S; \{n_i^{(k)}\}_{i=1...n_{\text{evts}}}^{(k)})$$

No overlaps between categories \Rightarrow No stat. correlations \Rightarrow product of PDFs.



Similar to a-posteriori combination but allows proper handling of correlated parameters (CR scale factors, systematics, etc.)

DDE for actor on l

Categories for $H \rightarrow \gamma \gamma$ Property Measurements

Categories also useful to provide measurements of separate kinematic regions \rightarrow e.g. differential cross-section measurements



Many categories, combined analysis for optimal use of all information

Systematics

Statistical model typically includes

- Parameters of interest (POIs) : S, σ×B, m_w, …
- Nuisance parameters (NPs) : other parameters needed to define the model

 \rightarrow Ideally, constrained by data like the POI

e.g. shape of $H \rightarrow \mu\mu$ continuum bkg

What about systematics ?

= what we don't know about the random process e.g. integrated luminosity L of a data sample for a cross-section measurement

\Rightarrow Parameterize using additional free parameters (NPs)

\rightarrow By definition, not constrained by the data

⇒ Cannot really be free parameters, or would spoil the measurement (*lumi free* ⇒ *no* σ ×*B measurement!*)

\Rightarrow Need to inject additional information

Phys. Rev. Lett. 119 (2017) 051802



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Frequentist Constraints

Prototype: NP measured in a separate *auxiliary* experiment e.g. luminosity measurement

 \rightarrow Build the combined PDF of the main+auxiliary measurements

 $P(\sigma, \theta_{lumi}; data) = P_{main}(\sigma, \theta_{lumi}; main data) P_{aux}(\theta_{lumi}; lumi data)$

Independent measurements: \Rightarrow just a product

Gaussian form often used by default: $L_{aux}(\theta; aux. data) = G(\theta^{obs}; \theta, \sigma_{syst})$

In the combined PDF, systematic NPs are constrained Systematics -> just additional NPs

→ Often no clear setup for auxiliary measurements
 e.g. theory uncertainties on missing HO terms from scale variations
 → Implemented in the same way nevertheless ("pseudo-measurement")

Likelihood, the full version (binned case)



× number of categories! 20

Model Example: $H \rightarrow \gamma \gamma$ Discovery Analysis



ATLAS Higgs Combination Model

parameters)

PANN

Atlas Higgs combination model (23.000 functions, 1600

Model has ~23.000 function objects, ~1600 parameters Reading/writing of full model takes ~4 seconds ROOT file with workspace is ~6 Mb

W. Verkerke, SOS 2014

F(x,p)

Computing Results

Using the PDF

Model describes the distribution of the observable: **P(data; parameters)** ⇒ Possible outcomes of the experiment, for given parameter values Can draw random events according to PDF : **generate (***pseudo-***)***data*



but not the main goal here

Likelihood

Model describes the distribution of the observable: $P(n; \lambda)$, P(data; parameters) \Rightarrow Possible outcomes of the experiment, for given parameter values We want the **other** direction: **use data to get information on parameters**



Likelihood: L(parameters) = P(data;parameters)

 \rightarrow same as PDF, but evaluated on data and function of the parameters

Estimating a Parameter: Maximum Likelihood



Going further: Hypothesis Testing

Hypothesis: assumption on model parameters, say value of S (e.g. H_n: S=O)

 \rightarrow Goal : determine if H₀ is true or false using a test based on the data

H₀ is false (New physics!)Discovery!Image: Missed discovery Type-II error (1 - Power)Image: Missed discovery Type-II error (1 - Power)H₀ is true (Nothing new)False discovery claim Type-I error (→ p-value, significance)Missed discovery Type-II error () No new physics, none foundImage: Missed discovery Type-II error () No new physics, none found	Possible outcomes:	Data disfavors H _o (Discovery claim)		Data favors H _o (Nothing found)	
$ \begin{array}{c} H_{0} \text{ is true} \\ (Nothing new) \end{array} \\ \hline H_{0} \text{ is true} \\ (nothing new) \end{array} \\ \hline H_{0} \text{ is true} \\ \hline $	H ₀ is false (New physics!)	Discovery!		Missed discovery Type-II error (1 - Power)	
	H _o is true (Nothing new)	False discovery claim Type-I error (→ p-value, significance)		No new physics, none found	Linearche services Linearche (Linearche) Linearche (Linearche) Li

Stringent discovery criteria ⇒ lower Type-I errors, higher Type-II errors → Goal: test that minimizes Type-II errors for given level of Type-I error.



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Possible outcomes:	Data disfavors H _o (Discovery claim)		Data favors H _o (Nothing found)	
H _o is false (New physics!)	Discovery!		Missed discovery Type-II error (1 - Power)	
H _o is true (Nothing new)	False discovery claim Type-I error (→ p-value, significance)		No new physics, none found	Image: Sector Secto
		0.4		

Stringent discovery criteria ⇒ lower Type-I errors, higher Type-II errors → Goal: test that minimizes Type-II errors for given level of Type-I error.



Hypothesis Testing with Likelihoods

Neyman-Pearson Lemma

When comparing two hypotheses, say $S=S_0$ and $S=S_1$, the optimal discriminator is the **Likelihood ratio** (LR)

 $\frac{L(S=S_1; data)}{L(S=S_0; data)}$

As for MLE, choose the hypothesis that is most likely **given the data**.

 \rightarrow Minimizes Type-II uncertainties for given level of Type-I uncertainties

Caveat: Strictly true only for *simple hypotheses* (no free parameters)

What about nuisance parameters ? (systematics, etc.)

Hypothesis Testing with Likelihoods

Profile Likelihood Ratio

When comparing two hypotheses, say $S=S_0$ and $S=S_1$, define the **Profile Likelihood ratio** (PLR) :

$$\frac{L(S=S_1, \hat{\hat{\theta}}(S_1); data)}{L(S=S_0, \hat{\hat{\theta}}(S_0); data)}$$

Again, use the value of the NP θ that is **most likely given the data** : **Profiling** Not guaranteed to be optimal, but works extremely well in practice

 \rightarrow In the following: all tests based on LR, will focus on p-values (Type-I errors), trusting that Type-II errors are anyway as small as they can be...

Discovery

Discovery :

- H₀: background only (S = 0) against
- H_1 : presence of a signal ($S \neq 0$)
- → For H_1 , any S≠0 is possible, which to use ? The one preferred by the data, \hat{S} .

$$\Rightarrow Use$$

$$t_0 = -2\log\frac{L(S=0, \hat{\theta}(S=0))}{L(\hat{S}, \hat{\theta})}$$



Why?

- \rightarrow Large values of $\dagger_0 \Leftrightarrow$ large observed S
- \rightarrow Gaussian limit (n_{obs} > 5): t₀ follows a χ^2 with n_{dof}=1, regardless of NPs!

 \rightarrow In particular,

$$Z=\sqrt{t_0}$$

Example: Gaussian Counting

Count number of events n in data

 \rightarrow assume n large enough so process is Gaussian

 $L(S:n) = e^{-\frac{1}{2}\left(\frac{n-(S+B)}{\sqrt{S+B}}\right)^2}$

 \rightarrow assume B is known, measure S

Likelihood :

$$\lambda(S;n) = \left(\frac{n - (S + B)}{\sqrt{S + B}}\right)^2$$

MLE for $S : \hat{S} = n - B$

Test statistic: assume $\hat{S} > 0$,

$$t_0 = -2\log\frac{\boldsymbol{L(S=0)}}{\boldsymbol{L(\hat{S})}} = \lambda(S=0) - \lambda(\hat{S}) = \left|\frac{n-B}{\sqrt{B}}\right|^2 = \left|\frac{\hat{S}}{\sqrt{B}}\right|^2$$

~

Finally:

$$Z = \sqrt{q_0} = \frac{S}{\sqrt{B}}$$

Known formula!

 \rightarrow Strictly speaking only

valid in Gaussian regimge



Example: Poisson Counting

Same problem but now not assuming Gaussianity

- $L(S;n) = e^{-(S+B)}(S+B)^n$ $\lambda(S;n) = 2(S+B) 2n\log(S+B)$
- MLE: $\hat{S} = n B$, same as Gaussian

Test statistic (for
$$\hat{S} > 0$$
): $q_0 = \lambda(S=0) - \lambda(\hat{S}) = -2\hat{S} - 2(\hat{S}+B) \log \frac{B}{\hat{S}+B}$

Assuming asymptotic distribution for q_0 ,

$$Z = \sqrt{2} \left[(\hat{S} + B) \log \left| 1 + \frac{\hat{S}}{B} \right| - \hat{S} \right]$$

Exact result can be obtained using pseudo-experiments \rightarrow close to $\sqrt{q_0}$ result

Asymptotic formulas justified by Gaussian regime, but remain valid even for small values of S+B (5!)



Some Examples

Higgs Discovery: Phys. Lett. B 716 (2012) 1-29



High-mass $X \rightarrow \gamma \gamma$ Search: JHEP 09 (2016) 1



Likelihood Intervals

Confidence intervals from L:

Test $H(\mu_{n})$ against alternative using

 $t_{\mu_0} = -2\log\frac{L(\mu = \mu_0)}{L(\hat{\mu})}$ Asymptotics: $t_{\mu} \sim \chi^2(N_{POI})$ under $H(\mu_0)$

In practice: $(N_{POI}=1)$

- Plot t_{..} vs. µ
- The minimum occurs at $\mu = \hat{\mu}$
- Crossings with $\mathbf{t}_{\mathbf{u}} = \mathbf{Z}^2$ give the **±**Zo uncertainties
- \rightarrow Gaussian case: parabolic profile,

$$t_{\mu} = \left(\frac{\mu - \hat{\mu}}{\sigma}\right)^2 \Rightarrow \mu_{\pm} = \hat{\mu} \pm \sigma \text{ at } t_{\mu} = 1$$

 \rightarrow robust against non-Gaussian effects.

 \rightarrow Can set upper limits on parameters using similar methods





µ can be

several POI!

2D Example: Higgs σ_{vBF} **vs.** σ_{ggF}

ATLAS-CONF-2017-047




Profiling : ttH→bb as an example

Analysis uses low-S/B categories to constrain backgrounds.

- \rightarrow Reduction in large uncertainties on tt bkg
- \rightarrow Propagates to the high-S/B categories through the statistical modeling
- ⇒ Care needed in the propagation (e.g. different kinematic regimes)



24 j, 2 b

2 5 j, 2 b

 $2 \ge 6 j, 2 b$

S/B = 0.1%

S/B = 0.1%

В

s/

В

S / \B

S/B = 0.0%

24 j, 3 b

2 5 j, 3 b

 $2 \ge 6 j, 3 b$

S/B = 1.3%

S/B = 0.6%

В

s/

Ш

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В

s/

S/B = 0.3%

В

S

В

Ś

В

S

24i.≥4b

 $25 i, \ge 4 b$

S/B = 3.6%

 $2 \ge 6 i \ge 4 b$

 $S/B = 5.2^{\circ}$

S/B = 2.2%

Profiling Issues

Too simple modeling can have unintended effects

 \rightarrow e.g. single Jet E scale parameter: \Rightarrow Low-E jets calibrate high-E jets – intended ?



Two-point uncertainties:

 \rightarrow Interpolation may not cover full configuration space, can lead to too-strong constraints



Profiling Issues

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Pull/Impact plots

ATLAS-CONF-2016-058

Critical to check syst modeling!

 \rightarrow Ongoing program

 \rightarrow Getting more important as syst uncertainties start to dominate

Example: pull/impact plots

Systematics NPs : usually

 $N = N_0 \left(1 + \sigma_{\text{syst}} \theta \right), \theta \sim G(0, 1)$

- central value = 0, → pre-fit expectation (usually MC)
 → If not: data/MC discrepancy ?
- uncertainty = 1 (normalized to the magnitude of the systematic)

→ If not: syst NP constrained by data
⇒ legitimate, or modeling issue ?

Impact on result of $\pm 1\sigma$ shift of NP



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Impact on result of $\pm 1\sigma$ shift of NP

13 TeV single-t XS (arXiv:1612.07231)



Pull/Impact plots

Critical to check syst modeling!

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Example: pull/impact plots

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Impact on result of $\pm 1\sigma$ shift of NP



1	2	3	4	8	18	33	30	25	0	9	20	35	8	35	25	10	13	33	0	0	0	100
3	4	6	10	23	-38	20	4	1	0	22	31	25	26	31	10	17	19	31	0	0	100	0
3	6	11	18	24	19	4	1	0	0	29	25	15	25	13	7	15	17	19	0	100	0	0
15	19	32	29	19	8	2	0	0	0	73	25	8	25	9	5	13	13	15	100	0	0	0
7	10	15	14	15	17	9	4	3	0	0	58	42	43	56	24	0	0	100	15	19	31	33
1	3	5	9	13	18	14	8	9	0	0	39	27	37	25	15	0	100	0	13	17	19	13
1	2	3	6	10	20	22	12	11	0	0	37	24	42	15	12	100	0	0	13	15	17	10
2	2	3	4	7	10	9	11	6	0	0	20	25	0	0	100	12	15	24	5	7	10	25
3	6	9	11	15	20	16	8	8	0	0	44	42	0	100	0	15	25	56	9	13	31	35
6	8	12	13	16	23	14	6	5	0	0	66	29	100	0	0	42	37	43	25	25	26	8
3	4	7	8	11	18	19	14	11	0	0	0	100	29	42	25	24	27	42	8	15	25	35
6	Э	e	SE	e r	4)n	0	T	K	e	SL	4.	S	37	39	58	25	25	31	20
12	16	29	31	30	22	9	4	2	0	100	0	0	0	0	0	0	0	0	73	29	22	9
71	38	27	11	_ 4	_ 1	_ 1	0	0	100	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	100	0	2	6	11	5	8	6	11	9	3	0	0	1	25
0	0	0	0	0	0	0	100	0	0	4	6	14	6	8	11	12	8	4	0	1	4	30
0	0	0	0	0	0	100	0	0	1	9	16	19	14	16	9	22	14	9	2	4	20	33
0	0	0	0	0		0	0	0	1	22	25	18	23	20	10	20	18	17	8	19	38	18
0	0	0	0	100	0	0	0	0	4	30	19	11	16	15	7	10	13	15	19	24	23	8
0	0	0	100	0	0	0	0	0	11	31	15	8	13	11	4	6	9	14	29	18	10	4
0	0	100	0	0	0	0	0	0	27	29	13	7	12	9	3	3	5	15	32	11	6	3
0		0	0	0	0	0	0	0	38	16	9	4	8	6	2	2	3	10	19	6	4	2
100	0	0	0	0	0	0	0	0	71	12	6	3	6	3	2	1	1	7	15	3	3	44

Reparameterization

Start with basic measurement in terms of e.g. $\sigma \times B$

 \rightarrow How to measure derived quantities (couplings, parameters in some theory model, etc.)? \rightarrow just reparameterize the likelihood:

e.g. Higgs couplings: σ_{qgF} , σ_{VBF} sensitive to Higgs coupling modifiers κ_{V} , κ_{F} .



Reparameterization: Limits

CMS Run 2 Monophoton Search: measured N_s in a counting experiment reparameterized according to various DM models





Presentation of Results

Measurements often recast to constrain a particular theory model.

 \rightarrow Ideally, by **reparameterizing the likelihood** and repeating the measurement



- \Rightarrow Done by experiments for selected benchmark models
- \rightarrow However, usually too complex to implement for many models

 \rightarrow Publishing full likelihood typically impractical – most theorists do not want to deal with 4000 NPs...

 \rightarrow Other approaches: e.g. reimplementing the analysis in a public fast-simulation framework (e.g. SUSY searches). However clear accuracy limitations

Presentation of Results

 \rightarrow **Current solution**: publish covariance matrices in HEPData, together with the individual measurements





\rightarrow Valid in the Gaussian approximation

- \rightarrow To go further, need some form of **simplified likelihoods**
- Profile likelihood function of POI only (NPs profiled out)
- Additional terms for non-Gaussian effects
- \rightarrow Significantly more complex (many dimensions!)
- \rightarrow Will be needed eventually as measurements become syst-dominated

Other Methods

BLUE

Commonly-used ansatz for combination of measurements:

1. **Build a x²:** (same as -2logL for Gaussian L)

$$\chi^{2}(X) = \sum_{i} \left(X_{i}^{\text{obs}} - X \right) C_{ij}^{-1} \left(X_{j}^{\text{obs}} - X \right)$$

2. Estimate combined X from minimum of $\chi^2(X)$

- In the Gaussian case, equivalent to ML solution
 → "Best" : minimizes the combined uncertainty
- Solution is a linear combination of the inputs:
- ⇒ "Best Linear Unbiased Estimator" (BLUE)

$$C_{ij}: \text{ covariance matrix of measurements:}$$

$$C = \begin{bmatrix} \sigma_1^2 & \rho \sigma_1 \sigma_2 & \cdots \\ \rho \sigma_1 \sigma_2 & \sigma_2^2 & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

$$\rho: \text{ correlation coefficients}$$

$$\boldsymbol{\lambda} = \frac{\boldsymbol{C}^{-1} \boldsymbol{J}}{\boldsymbol{J}^{T} \boldsymbol{C}^{-1} \boldsymbol{J}}, \ \boldsymbol{J} = \begin{vmatrix} 1 \\ 1 \\ \vdots \end{vmatrix}$$

 λ_i = combination weight of measurement i

$$\hat{X} = \sum_{i} \lambda_{i}^{\dagger} X^{obs, i}$$

BLUE Example

ATLAS-CONF-2014-008







Limitation: relies on **Gaussian assumptions** (satisfied in this case!) Non-trivial results for strong correlations, see Eur. Phy. J. C 74 (2014), 2717)

Uncertainty decomposition



Uncertainty decomposition



Frequentist vs. Bayesian

All methods described so far are frequentist

- Probabilities (p-values) refer to outcomes if the experiment were repeated identically many times
- Parameters value are fixed but unknown
- Probabilities apply to measurements:
- \rightarrow "m_H = 125.09 ± 0.24 GeV" :



 \rightarrow i.e. [125.09 - 0.24 ; 125.09 + 0.24] GeV has p=68% to contain **the** true m_H.

 \rightarrow if we repeated the experiment many times, we would get different intervals, 68% of which would contain the true $\rm m_{\rm H^{-}}$

\rightarrow "5 σ Higgs discovery"

• if there is really no Higgs, such fluctuations observed in 3.10⁻⁷ of experiments

Not exactly the crucial question – what we would really like to know is What is the probability that the excess we see is a fluctuation → we want P(no Higgs | data) – but all we have is P(data | no Higgs)

Frequentist vs. Bayesian



Can compute $P(\mu \mid data)$, if we provide $P(\mu)$

- \rightarrow Implicitly, we have now made μ into a random variable
 - Is m_{H} , or the presence of H(125), randomly chosen ?
 - In fact, different definition of p: *degree of belief*, not from frequencies.
 - $P(\mu)$ **Prior degree of belief** critical ingredient in the computation

Compared to frequentist PLR: • answers the "right" question • answer depends on the prior "Bayesians address the questions everyone is interested in by using assumptions that no one believes. Frequentist use impeccable logic to deal with an issue that is of no interest to anyone." - **Louis Lyons**

What was the question ?

Definition of the p-value:



p-value = $\frac{\text{number of signal-like outcomes with only background present}}{\text{all outcomes with only background present}}$

So 5 σ significance ($p_n \sim 10^{-7}$) \Leftrightarrow Occurs once in 10⁷ if only background present

However this is **NOT** "*One chance in 10⁷ to be a fluctuation*"

The first statement is about **data probabilities** – **P(data; H_n)**

The second is on $P(H_0)$ itself – not addressed in the framework described so far \rightarrow makes sense in a **Bayesian** context.

It's also a different statement (although they sometimes get confused) \rightarrow If a signal outcome is also very unlikely, we may not want to reject H₀, even with p₀ ~ 10⁻⁷.

What was the question ?

e.g. Faster-than-light neutrino anomaly

 $(v-c)/c = (2.37 \pm 0.32 \text{ (stat.)} ^{+0.34}_{-0.24} \text{ (sys.)}) \times 10^{-5}$ 6.20 above c

"despite the large significance of the measurement reported here and the stability of the analysis, the potentially great impact of the result motivates the continuation of our studies in order to investigate possible still unknown systematic effects that could explain the observed anomaly."

⇒ Very unlikely to be a background fluctuation, but hard to believe since alternative (v>c) is far-fetched



"Extraordinary claims require extraordinary evidence"

Alternative: $P(\text{fluctuation}) = \frac{\text{number of signal-like outcomes with only B present}}{\text{number of signal-like outcomes from any source (S or B)}}$ $= \frac{P(\text{deviation}|B)P(B)}{P(\text{deviation}|S)P(S) + P(\text{deviation}|B)P(B)}$

- \rightarrow Needs *a priori* P(S) and P(B) \rightarrow Bayesian methods
- \rightarrow In frequentist context, only have $\mathbf{p}_0 = \mathbf{P}(\mathbf{deviation} \mid \mathbf{B})$
- \Rightarrow However usually same conclusion, assuming P(S) is not $\ll p_0...$

Expected Sensitivity



Expected Results

Expected results: median outcome under a given hypothesis

 \rightarrow e.g. SM case, background only, etc

Two main ways to compute:

 \rightarrow **Pseudo-experiments**: use statistical model to generate pseudo-data ("toy data"),

→ Asimov Datasets

- Generate a "perfect dataset"
 e.g. for binned data, each bin set to expectation:
- Gives the median result immediately:
 median(toy results) ↔ result(median dataset)
- Get bands from asymptotic formulas: Band width $\sigma_{0}^{2} = \frac{S_{0}^{2}}{1-S_{0}^{2}}$

$$a_{S_0,A}^2 = \frac{B_0}{q_{S_0}(\text{Asimov})}$$

⊕ Much faster (1 "toy")

⊖ Relies on Gaussian approximation





59

Expected Limits

1D: Asimov & toys give similar results → Asimov used in most cases
 2D: Different results: "Typical" and "Median" exclusion do not match!
 →Asimov still preferred since "typical" is usually more relevant.



60

Look-Elsewhere Effect



Look-Elsewhere effect

Sometimes, unknown parameters in signal model

e.g. p-values as a function of $\rm m_{\rm x}$

⇒ Effectively performing **multiple, simultaneous** searches

→ If e.g. small resolution and large scan range, **many independent experiments**



Probability for a fluctuation:

anywhere in the range at a given location



→ More likely to find an excess **anywhere in the range**, rather than in a **predefined** location

⇒ Look-elsewhere effect (LEE)

- \rightarrow **Global** significance
- \rightarrow Local significance ₆₂

Global Significance

$$\begin{array}{c|c} \textbf{Global} & \textbf{p}_{global} = 1 - (1 - p_{local})^{N}_{\textbf{A}} \approx N p_{local} & \textbf{Local} \\ \hline \textbf{p-value} & \textbf{Trials factor} & \textbf{p-value} \\ \hline \textbf{Trials factor} & \textbf{p}_{local} \Rightarrow \textbf{p}_{lo$$

Trials factor : **naively** = # of independent intervals: However this is usually **wrong**

??
$$N_{\text{trials}} \equiv N_{\text{indep}} = \frac{\text{scan range}}{\text{peak width}}$$

Gross & Vitells EPJC 70:525-530,2010

Actually,
$$N_{\text{trials}} = 1 + \sqrt{\frac{\pi}{2}} N_{\text{indep}} Z_{\text{local}}$$

(1 POI, asymptotic limit)

Can also use brute-force toys:

Generate toys \Rightarrow find such an excess 2% of the time $\Rightarrow p_{global} \sim 2 \ 10^{-2}$, $Z_{global} = 2.1\sigma$ Less exciting...





Machine Learning

Old idea, now reaching maturity in HEP applications. Main example is **neural networks**:



- \rightarrow many neurons per layer
- Made possible by
- \rightarrow **Increased computing power** (e.g. GPUs)

 \rightarrow **New methods** : Cross-entropy training (same as max. likelihood), dropout, non-sigmoid activation functions, etc.) to improve training performance

Machine Learning Discriminants

Usual statistical methods work well for

- → Event counting
- → 1D distributions
- ML : Build discriminant, → use in 1D shape analyses

Already in common use (e.g. BDTs)

DNNs:

- \rightarrow Better performance
- \rightarrow Can work on low-level inputs (4-vectors)

 \Rightarrow No need for "hand-crafted" variables

- Θ Still can't do better than Likelihood ratio
- Can provide arbitrarily good approximations!



Signal efficiency

66

P. Baldi, P. Sadowski & D. Whiteson, Nature Comm. vol. 5, 4308 (2014)

ML Computing Backends

ML computing-intensive ⇒ efficient implementations: e.g. TensorFlow, PyTorch

 \rightarrow Parallelization, use of GPU architecture

→ New techniques: e.g. automatic gradient computations

ATLAS: pyhf, reimplementation of ROOT-based HistFactory framework

CMS: TF implementation of combine code





	Likelihood	${\sf Likelihood}{+}{\sf Gradient}$	Hessian
Combine, TR1950X 1 Thread	10ms	830ms	-
TF, TR1950X 1 Thread	70ms	430ms	165s
TF, TR1950X 32 Thread	20ms	71ms	32s
TF, 2x Xeon Silver 4110 32 Thread	17ms	54ms	24s
TF, GTX1080	7ms	13ms	10s
TF, V100	4ms	7ms	8s

J. Bendavid



Other Applications

Many other applications:

Convolutive neural networks (CNNs)

 \rightarrow "computer vision" : treat physics objects as images

 \Rightarrow Ideal for future high-granularity detectors

Recurrent NNs (RNNs)

 \rightarrow language processing : treat collections of objects (tracks, cluster, cells) as sentences

Adversarial NNs

 \rightarrow trained in pairs to optimize against systematics, or data/MC differences.







JHEP 07 (2016) 069

Factors 100-1000 gain in shower simulation time



Generative Adversarial Network (GAN)

Liquid State Machine (LSM) Extreme Learning Machine (ELM)

Echo State Network (ESN)

Conclusion

New developments in statistical methods in the last decade or so
 → Baseline methods reaching maturity

- Many challenges still to be addressed
 - \rightarrow Modeling complex experiments (systematics)
 - \rightarrow Pusblishing data to allow efficient re-interpretation

 \rightarrow ...

New horizons going towards machine learning

Books and Courses



Some courses available online:

Glen Cowan's Cours d'Hiver and 2010 CERN Academic Training lectures Kyle Cranmer's CERN Academic Training lectures Louis Lyons'and Lorenzo Moneta's CERN Academic Training Lectures

Extra Material
BLUE and PLR

PLR Computation: 2 measurements + 1 auxiliary measurement

$$X_{1} = X + \Delta_{1} \theta \sim G(X^{*}, \sigma_{1})$$
$$X_{2} = X + \Delta_{2} \theta \sim G(X^{*}, \sigma_{2})$$
$$\theta \sim G(0, 1)$$

Single measurement:
$$\lambda(X,\theta) = \frac{1}{\sigma_1^2} (X + \Delta_1 \theta - X_1^{\text{obs}})^2 + (\theta - \theta^{\text{obs}})^2$$
$$MLES: \begin{cases} \hat{\theta} = \theta^{\text{obs}} \\ \hat{\theta} = \theta^{\text{obs}} \\ \hat{X} = X_1^{\text{obs}} - \Delta_1 \theta^{\text{obs}} \\ PLR: \quad \lambda(X) = \frac{(X - \hat{X})^2}{\sigma_{1, \text{tot}}^2} \qquad \sigma_{1, \text{tot}}^2 = \sigma_1^2 + \Delta_1^2$$
$$Combination: \quad \lambda(X,\theta) = \frac{1}{\sigma_1^2} (X + \Delta_1 \theta - X_1^{\text{obs}})^2 + \frac{1}{\sigma_2^2} (X + \Delta_2 \theta - X_2^{\text{obs}})^2 + (\theta - \theta^{\text{obs}})^2$$

MLE:
$$\hat{X} = \lambda_1 X_1^{\text{obs}} + \lambda_2 X_2^{\text{obs}} + \lambda_{\theta} \theta^{\text{obs}}$$
 $\lambda_{1(2)} = \frac{\sigma_{2(1), \text{tot}}^2 - \Delta_1 \Delta_2}{\sigma_{1, \text{tot}}^2 + \sigma_{2, \text{tot}}^2 - 2\Delta_1 \Delta_2}$

PLR:
$$\lambda(X) = \frac{(X - \hat{X})^2}{\sigma_{X, \text{tot}}^2}$$
 $\sigma_{X, \text{tot}}^2 = \frac{\sigma_{1, \text{tot}}^2 \sigma_{2, \text{tot}}^2 - \Delta_1^2 \Delta_2^2}{\sigma_{1, \text{tot}}^2 + \sigma_{2, \text{tot}}^2 - 2\Delta_1 \Delta_2}$

BLUE and PLR

BLUE computation: measurements X_1 and X_2 with uncorrelated statistical uncertainties σ_1 and σ_2 , correlated systematics Δ_1 and Δ_2 . Single measurement: stat uncertainty σ_1 , systematic Δ_1 - Uncorrelated uncertainties - Assume everything is Gaussian ⇒ Uncertainties add $\sigma_{1 \text{ tot}}^2 = \sigma_1^2 + \Delta_1^2$ in quadrature: $C = \begin{bmatrix} \sigma_{1, \text{ tot}}^2 & \rho \sigma_{1, \text{ tot}} \sigma_{2, \text{ tot}} \\ \rho \sigma_{1, \text{ tot}} \sigma_{2, \text{ tot}} & \sigma_{2, \text{ tot}}^2 \end{bmatrix} \quad \rho = \frac{\Delta_1 \Delta_2}{\sigma_{1, \text{ tot}} \sigma_{2, \text{ tot}}}$ **Combination**: $\lambda_{1(2)} = \frac{\sigma_{2(1), \text{tot}}^2 - \rho \sigma_{1, \text{tot}} \sigma_{2, \text{tot}}}{\sigma_{1}^2 + \sigma_{2}^2 - 2\rho \sigma_{1, \text{tot}} \sigma_{2, \text{tot}}}$ **BLUE** weights $\hat{X} = \lambda_1 X_1^{obs} + \lambda_2 X_2^{obs}$ Propagate uncertainties from C: $\sigma_{X, \text{tot}}^2 = \frac{\sigma_{1, \text{tot}}^2 \sigma_{2, \text{tot}}^2 (1 - \rho^2)}{\sigma_{1, \text{tot}}^2 + \sigma_{2, \text{tot}}^2 - 2\rho\sigma_{1, \text{tot}}\sigma_{2, \text{tot}}^2}$

Beyond Asymptotics: Toys

Asymptotics usually work well, but break down in some cases – e.g. small event counts.

Solution: generate *pseudo data* (toys) using the PDF, under the tested hypothesis

 \rightarrow Also randomize the observable

PDF

120

130

140

150

m (GeV)

160

Vormalized events per GeV

0.025

0.02

0.015

0.01

0.005

100

110

(**9**^{obs}) of each auxiliary experiment:

 \rightarrow Samples the true distribution of the PLR

 \Rightarrow Integrate above observed PLR to get the p-value \rightarrow Precision limited by number of generated toys, Small p-values ($5\sigma : p \sim 10^{-7}!$) \Rightarrow large toy samples

3000

2500

2000

1500

1000

500

100

Vormalized events per GeV

p(data|x)

CMS-PAS-HIG-11-022



m (GeV)

Toys: Example

ATLAS X \rightarrow Z γ Search: covers 200 GeV < m_x < 2.5 TeV \rightarrow for m_x > 1.6 TeV, low event counts \Rightarrow derive results from toys



Asymptotic results (in gray) give optimistic result compared to toys (in blue)

Rare Processes

HEP : almost always rare processes

ATLAS :

- Event rate ~ 1 GHz (L~10³⁴ cm⁻²s⁻¹~10 nb⁻¹/s, σ_{tot} ~10⁸ nb,)
- Trigger rate ~ 1 kHz

(Higgs rate ~ 0.1 Hz) $\Rightarrow P \sim 10^{-6} \ll 1 (P_{H \rightarrow W} \sim 10^{-13})$

A day of data: $N \sim 10^{14} \gg 1$

Large N, small $P \Rightarrow$ Poisson regime!

(Large N = design requirement, to get not-too-small λ =NP...)



Asymptotic Approximation: Wilks' Theorem

 \rightarrow Assume **Gaussian regime for Ŝ** (e.g. large n_{evts})

 \Rightarrow Central-limit theorem :

 t_0 is distributed as a χ^2 under the hypothesis H_0

 $f(t_0 \mid H_0) = f_{\chi^2(n_{dof}=1)}(t_0)$

In particular, significance:

$$Z = \sqrt{t_0} \qquad \qquad \begin{array}{c} \text{By definition,} \\ t_0 \sim \chi^2 \Rightarrow \sqrt{t_0} \sim G(0,1) \end{array}$$

Typically works well for for event counts O(5) and above (5 already "large"...)

The 1-line "proof": asymptotically L and S are Gaussian, so

$$L(S) = \exp\left[-\frac{1}{2}\left(\frac{S-\hat{S}}{\sigma}\right)^2\right] \Rightarrow t_0 = \left(\frac{\hat{S}}{\sigma}\right)^2 \Rightarrow t_0 \sim \chi^2(n_{dof} = 1) \text{ since } \hat{S} \sim G(0, \sigma)$$



Cowan, Cranmer, Gross & Vitells Eur.Phys.J.C71:1554,2011

 $t_0 = -2\log\frac{L(S=0)}{L(\hat{S})}$

78

Intervals

If $\hat{\mu} \sim G(\mu^*, \sigma)$, known quantiles :

 $P(\mu^* - \sigma < \hat{\mu} < \mu^* + \sigma) = 68\%$

This is a probability for $\hat{\mu}$, not μ ! $\rightarrow \mu^*$ is a fixed number, not a random variable

But we can invert the relation:

$$P(\mu^* - \sigma < \hat{\mu} < \mu^* + \sigma) = 68\%$$

$$\Rightarrow P(|\hat{\mu} - \mu^*| < \sigma) = 68\%$$

$$\Rightarrow P(\hat{\mu} - \sigma < \mu^* < \hat{\mu} + \sigma) = 68\%$$



→ This gives the desired statement on μ^* : *if we repeat the experiment many times,* $[\hat{\mu} - \sigma, \hat{\mu} + \sigma]$ will contain the true value 68% of the time: $\hat{\mu} = \mu^* \pm \sigma$ This is a statement on the interval $[\hat{\mu} - \sigma, \hat{\mu} + \sigma]$ obtained for each experiment

Works in the same way for other interval sizes: $[\hat{\mu} - Z\sigma, \hat{\mu} +]Z\sigma$ ith



Systematics NPs

Each systematics NP represent **an independent source of uncertainty** → Usually constrained by a single 1-D PDF (Gaussian, etc.)

Sometimes multiple parameters **conjointly constrained** by an n-dim. PDF. \rightarrow multiple measurements constraining multiple NPs

Assume n-dim Gaussian PDF: then can diagonalize the covariance matrix C and re-express the uncertainties in basis of eigenvector NPs \Rightarrow n 1-dim PDFs

Can also diagonalize to **prune** irrelevant uncertainties: keep NPs with large eigenvalues, combine in quadrature the others



Global Significance from Toys



Principle: repeat the analysis in toy data:

- \rightarrow generate pseudo-dataset
- → perform the search, scanning over parameters as in the data
- \rightarrow report the largest significance found
- \rightarrow repeat many times

 \Rightarrow The frequency at which a given Z₀ is found **is** the global p-value

e.g. X \rightarrow yy Search: Z_{local} = 3.9 σ (\Rightarrow p_{local} ~ 5 10⁻⁵), scanning 200 < m_x< 2000 GeV and 0 < Γ_x < 10% m_x

→ In toys, find such an excess 2% of the time ⇒ $p_{global} \sim 2 \ 10^{-2}$, $Z_{global} = 2.1 \sigma$ Less exciting...

Exact treatment

 Θ CPU-intensive especially for large Z (need ~O(100)/p_{global} toys)

Global Significance from Asymptotics

Principle: approximate the global p-value in the asymptotic limit \rightarrow reference paper: Gross & Vitells, EPJ.C70:525-530,2010

Asymptotic trials factor (1 POI):

→ Trials factor is **not just N**_{indep}, also depends on Z_{local} !

Why?

- \rightarrow slice scan range into $\rm N_{indep}$ regions of size ~ peak width
- \rightarrow search for a peak in each region
- \Rightarrow Indeed gives N_{trials}=N_{indep}.

However this misses peaks sitting on edges between regions

 \Rightarrow true N_{trials} is > N_{indep}!



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Illustrative Example

- Test on a simple example: generate toys with
- \rightarrow flat background (100 events/bin)
- \rightarrow count events in a fixed-size sliding window, look for excesses

Two configurations:

- 1. Look only in 10 slices of the full spectrum
- 2. Look in any window of same size as above, anywhere in the spectrum



Illustrative Example (2)

Very different results if the excess is **near a boundary :**



1. Look only in 10 slices of the full spectrum

2. Look in any window of same size as above, anywhere in the spectrum

Illustrative Example (3)



Classic Discoveries (1)

ĪŢ

1.55 1.552 1.554 1.556

1000

ADRANG

21

C.

8

100

20

scale

00





c

100

mete-

90

80

110

(GeV)

Discovery ψ

In this graph, the blue data points show a sharp peak in the number of hadrons produced at a narrow range of energies – evidence of the J/Ψ particle. The horizontal axis shows the energy of one of the pair of SPEAR beams, measured in GeV. The height of the peak is so great that, to fit the plot on one sheet of graph paper, the vertical axis is compressed into a logarithmic scale.

Huge signal S/B~50 Several 1000 events

1.56

1.57

Classic Discoveries (2)

OB:20 SON OF GLORY Church Mondrem, Allen Little, Bob Stega Jo it a

NOTES THE RESCAN (RAN 1922) WAS SHELLED AT "1975" DEALINED BY RUMMEN'S SOME NOOM 1.463, SO EUROPENES (DAL'S DON'T CREATING TO MELL AT LINE 1922

15 STOP. DUMP | Rick)

- WIE Preside on it 1,217 -
- Much has compared provides as into face. That I shared
- 30 DAMN LINAL RACE UP. DUMP + DIAN.



ψ' : discovered online by the (lucky) shifters



First hints of top at D0: O(10) signal events, a few bkg events, 2.4 σ

And now ?

Short answer: The high-signal, low-background experiments have been done already (although a surprise would be welcome...) *e.g.* at LHC:

- High background levels, need precise modeling
- Large systematics, need to be described accurately
- Small signals: need optimal use of available information :
 - Shape analyses instead of counting
 - Categories to isolated signal-enriched regions



Discoveries that weren't

UA1 Monojets (1984)

Volume 139B, number 1,2

PHYSICS LETTERS

3 May 1984

energy can be due either to: (i) One or more prompt neutrinos. (ii) Any invisible \mathbb{Z}^0 , such as $\mathbb{Z}^0 \to \nu\overline{\nu}$ decay, which is expected to have a large (18%) branching ratio. Note that the corresponding decays into charged lepton pairs $\mathbb{Z}^0 \to e^+e^-, \mathbb{Z}^0 \to \mu^+\mu^-$ have lower branching ratios (-3%) and may not have yet been produced within the present statistics.

At the present time we can only speculate about the origin of this new effect. The missing transverse

(iii) New, non-interacting neutral particles. The jets appear somewhat narrower and with lower multiplicities than the corresponding QCD jets, although it might be premature to draw conclusions on such limited statistics.

A number of theoretical speculations [9] may be elevant to these results. We mention briefly the possibilities of excited quarks or leptons and of composite or coloured or supersymmetric W's and Higgs. A re cent calculation [10] +8 has been made in the context of the present collider experiment, on the rate of event with large missing transverse energy from gluino pair production with each gluino decaying into a quark, antiquark, and photino. The non-interacting photinos may produce large apparent missing energy. For instance, the calculation gives an expectation of about 100 single-jet events with $\Delta E_{\rm M} > 20$ GeV for a gluino mass of 20 GeV/c2. Taking our excess of 5 events above background as an upper limit for such a process, we deduce that the gluino mass must be greater than about $40 \text{ GeV}/c^2$

EXPERIMENTAL OBSERVATION OF EVENTS WITH LARGE MISSING TRANSVERSE ENERGY ACCOMPANIED BY A JET OR A PHOTON (S) IN pp COLLISIONS AT \sqrt{s} = 540 GeV

UA1 Collaboration, CERN, Geneva, Switzerland

Pentaquarks (2003)



BICEP2 B-mode Polarization (2014)



Avoid spurious discoveries!

 \rightarrow Treatment of modeling uncertainties,

systematics in general

Phys. Rev. Lett. 91, 252001 (2003)

CaloGAN



FIG. 4: Composite Generator, illustrating three stream with attentional layer-to-layer dependence.



FIG. 5: Composite Discriminator, depicting additional domain specific expressions included in the final feature space.

M. Paganini et al., 1705.02355

Generation Method	Hardware	Batch Size	milliseconds/shower
GEANT4	CPU	N/A	1772 🛶 🔤
CALOGAN	CPU	1	13.1
		10	5.11
		128	2.19
		1024	2.03
	GPU	1	14.5
		4	3.68
		128	0.021
		512	0.014
		1024	0.012 ┥